A simulation of hard spheres gas for educational purposes

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Abstract. We describe an educational simulation of some effects within the gas of
hard spheres. The focus of the presented simulation is on the comprehension of random
character of the velocity of molecules in the gas and of the energy at fixed temperature.
It allows to point out the connection between the temperature, the energy, and the
velocity of the molecules.

1. Introduction

Thermodynamics and statistical physics provide the key to understanding many
physics phenomena and are therefore very important part of the secondary school
physics curriculum. A difficulty in their thorough understanding together with the
corresponding formulae is in the statistical treatment of a large number of atoms or
molecules. Quantities like *internal energy* or *mean quadratic velocity* are given by the
averages of those atributed to individual molecules. Internal energy is connected with
the temperature.

The averaging is based on the underlying Maxwell-Boltzmann distribution. It goes
beyond the secondary school curriculum to formally show, that this is the distribution
which does not change in time under influence of the collisions among the molecules.
Moreover, most distributions of the momenta of molecules will converge to Maxwell-
Boltzmann form as a result of molecular collisions.

We present here a simulation applet which explains these features of
thermodynamics without the need of formal mathematical formulae. The topic of using
applets for teaching physics is widely discussed in the literature, see e.g. [1] and [2] and
references therein. There are many simulations and applets, some also available on the
web, e.g. [3, 5, 4]. The teacher can choose among them if he or she wants to support
the explanation in the classroom or refer the pupils to some supporting material. It
is a matter of appropriatness to the particular topic which is being explained. In our

simulations we have put emphasis on i) explaining the correspondence between gas energy and mean quadratic velocity calculated from the temperature and those really measured—if this was possible on individual molecules; and ii) explain the random nature of the velocities of the molecules.

Our simulations are freely available on the web [6]

2. Ideal gas relations

The simulation shows *two-dimensional* gas of 500 single-atom molecules. Collisions of atoms are treated as elastic collisions of circles; this determines the angle of scattering and the outgoing momenta. Thus, strictly speaking, the gas is not ideal but rather described by the van der Waals equation of state. It is dilute, however, so that ideal gas relations can be applied. Collisions with the walls of the container are elastic, except for one wall which can be "heated".

We chose to perform the simulation in two dimensions since in such a case we can show all molecules straightforwardly and do not need to do any projections to a plane, which might be confusing. On the other hand, we have to keep in mind that this changes some relations. The (mean) internal energy of the gas is

$$E = \frac{2}{2} N \, k_B \, T \,, \tag{1}$$

where N is the number of atoms, T is the temperature and k_B the Boltzmann constant. Intentionally we display the factor 2/2—instead of 3/2—indicating that we are in two dimensions. Correspondingly, the relation for mean quadratic velocity reads

$$v = \sqrt{\frac{2 \, k_B \, T}{m}} \,, \tag{2}$$

where m is the mass of the atom and the factor 2 is due to two dimensions. Velocities are distributed according to the Maxwell distribution, which in two dimensions takes the form

$$\mathcal{P}(v_x, v_y) = \frac{m}{2\pi \, k_B \, T} \exp\left(-\frac{m(v_x^2 + v_y^2)}{2 \, k_B \, T} \right) . \tag{3}$$

3. The simulation

The simulation always shows a rectangular container with the gas. The color of the atom is chosen from a spectrum between blue (slow atoms) and red (fast atoms). In Figure 1 we show how the simulation looks like. Three of the sides always bounce off the atoms elastically.

One side can be made into a heater/cooler. In that case, its temperature can be set to some value. When the atoms bounce off this side, their velocity is determined randomly according to Maxwell distribution (eq. (3)) with the temperature parameter set to that of the heater/cooler and direction inwards the containter.
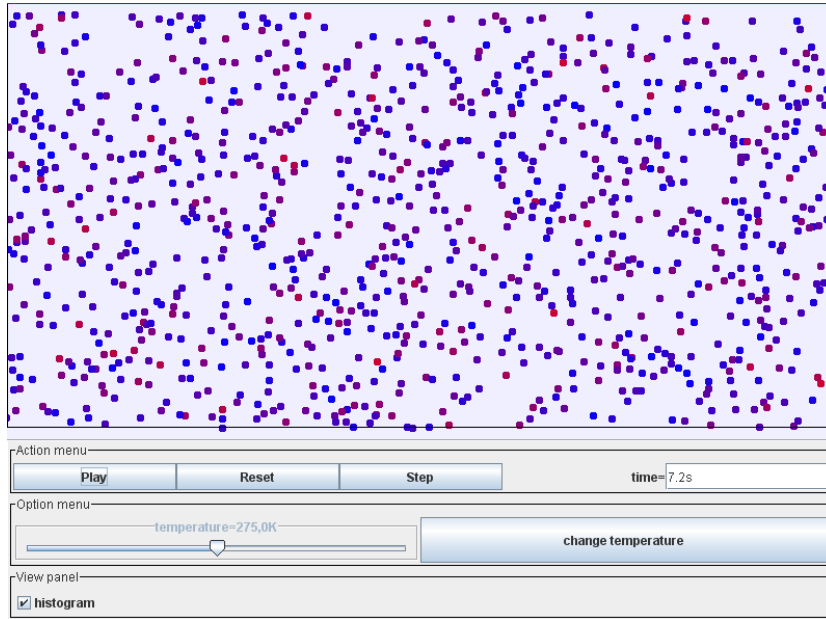
Figure 1. A typical simulation at high temperature; here the temperature is set to 500 K. At lower temperature there are less red (fast) atoms.

In a different setting, one of the sides is replaced by a piston which can be moved eigter by pressing arrow buttons in the simulation window or by clicking a draging.

Additional windows can be displayed. One of them contains the histogram of the velocity distribution which is updated in real time. Another one shows the graph of the time dependence of the gas energy compared with the value which the energy is expected to have according to the temperature of the heated wall. In the last auxilliary window the values of the actual energy, expected energy and mean quadratic velocity are displayed. The temperature ranges between 50 and 500 K and the typical velocities are of the order of hundreds of m.s^{-1}. With 500 atoms the typical energy is of the order of few electronvolts.

4. The presented effects

4.1. Velocity distribution

The simulation can be initiated in such a way that each atom has exactly the velocity v given by eq. (2), with random direction. During initialisation one time step is effectively performed and some collisions can occur, thus some velocities may slightly change. Nevertheless, the initial velocity histogram shows just one very narrow peak (Figure 2 left). The simulation can then be started and the user can observe how the velocity distribution quickly broadens and becomes maxwellian as a result of the collisions, see Fig. 2. It is interesting to run the simulation step by step since the process is very quick.
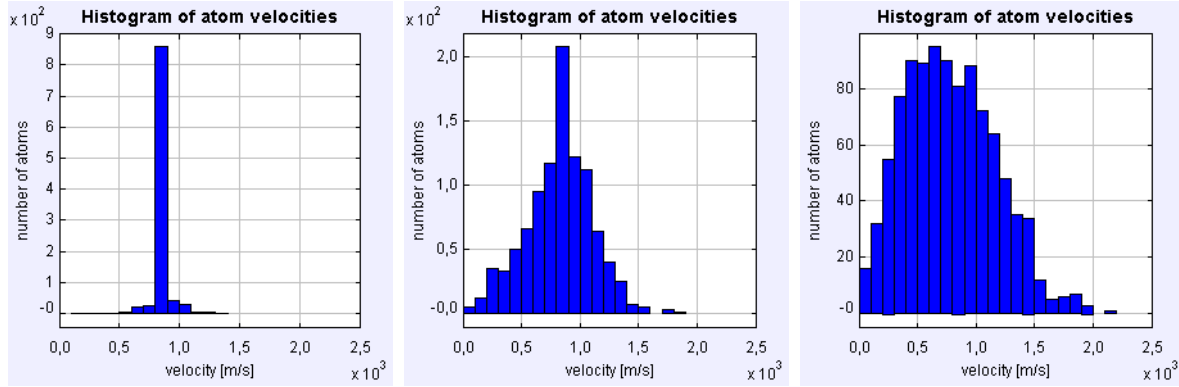
Figure 2. The influence of collisions of the distribution of velocities. Left is the initial distribution at time 0, in the middle is the histogram after 0.5 s, on the right the distribution after 2 s. After 2 s the histogram fluctuates but does not change its gross shape, if the temperature is kept constant.
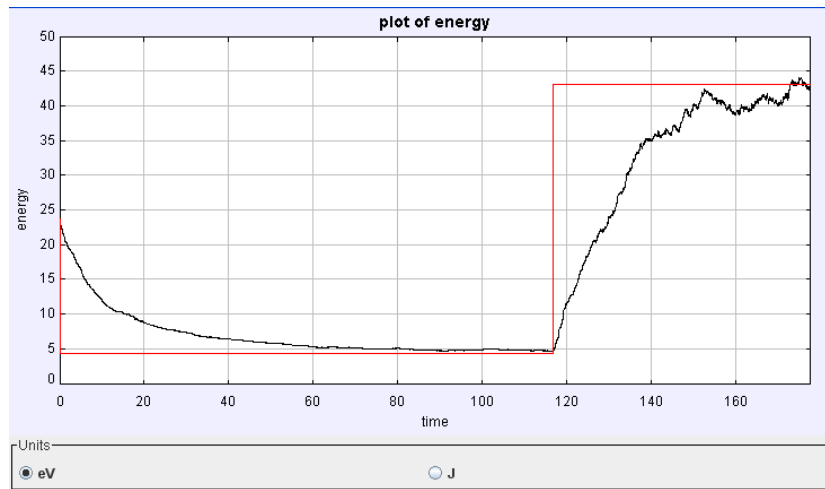

Figure 3. The red straight line shows the expected energy of the gas corresponding to the temperature of the heating wall. The black fluctuating line is the actual energy as a function of the time. The original temperature of the gas was 250 K. In the beginning the temperature of the heating/cooling wall was set to 50 K. After 100 s it was put to the value of 500 K.

4.2. Heating and cooling

In this mode of the simulation, one of the walls of the container can be set to a temperature different from that of the gas. Then is is interesting to observe the plot of the time dependence of the gas energy, which we show in Figure 3. It shows the expected value corresponding to the temperature of the heating or cooling wall, and the actual energy of the gas obtained by summing up kinetic energies of all atoms. On average, the actual energy converges to the expected one, and thermal fluctuations are clearly visible.

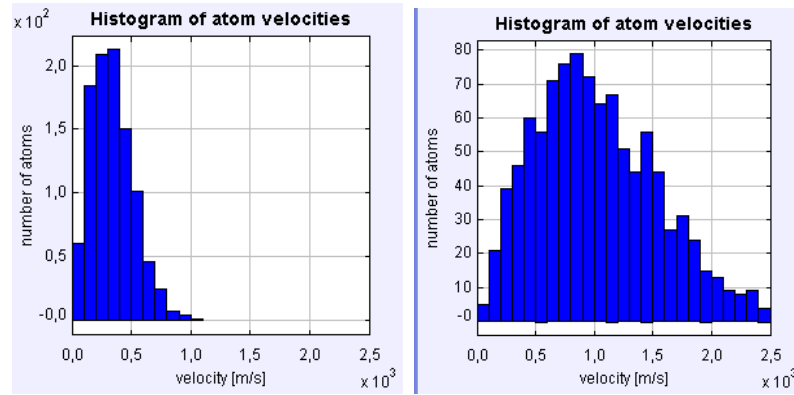It is also interesting to observe the velocity histogram (Figure 4). Here one can

Figure 4. The histograms of velocity distribution at the temperature of 50 K (left) and 500 K (right).

realise the connection between the temperature, the energy, and the distribution of velocities. It can be seen how the distribution broadens and the peak of the histogram (the most probable velocity) moves to higher values with increasing temperature, and vice versa, lower temperature leads to narrower histogram with a peak at lower velocity.

4.3. Pressing

One can also demonstrate the effect of pressing and releasing of the gas. One of the sides of the container is then turned into a piston. The piston should be moved slowly—slower than the typical velocity of the atoms. Otherwise the presentation is somewhat unrealistic. One can see that when the piston is pressing the volume, atoms are bounced off it with higher velocity than they had before and this increases the energy of the gas. This can be observed in the plot of energy as a function of time and on the velocity histogram. Increasing the volume with the help of the piston leads to the inverse effect.

4.4. Brownian motion

We have also prepared a simulation of the Brownian motion. Two larger circles with masses hundred times larger than the atoms are immersed into the gas which is initiated at the temperature of 250 K. As a result of the collisions they begin to move. The trajectory they have passed is shown in the simulation (Figure 5). One can also monitor their distance from the initial position as a function of time in a dedicated window.

5. Conclusions

We believe that our simulations can serve as a valuable supporting tool for explaining some features of the ideal gas. We plan to enlarge the collection of the addressed effects in the future.
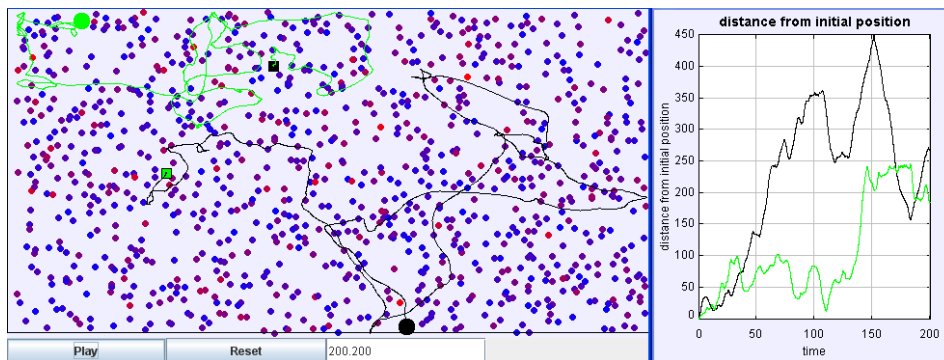
Figure 5. The simulation of Brownian motion. Paths of the two heavy particles are shown. In the separate window, their distance from the original position as a function of time is presented.

References

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